National Exams December 2005

98-Met-A4, Structure of Materials

<u>3 Hours Duration</u>

<u>NOTES:</u>

1. If doubt exists as to the interpretation of any question, the candidate is urged to submit with the answer paper, a clear statement of any assumptions made.

2. Candidates may use one of two calculators, the Casio or Sharp approved models. This is a Closed Book exam. All equations, constants and diagrams are given in the appendix.

3. **Any five** questions constitute a complete paper. **Only the first five questions** as they appear in your answer book will be marked.

4. All questions are of equal value.

Question I: Electron Structure

1. Four quantum numbers can be used to uniquely specify the state of each electron in an atom. List each of these four parameters and briefly explain what they describe. **(8 marks)**

2. Give the set of 4 possible quantum numbers for the outermost (valence) electron in Br^{-1}. Bromine has atomic number 35. **(6 marks)**

3. Phosphorous (Z=15) is polyvalent. It can form ions of charge: -3, +3, and +5. Give the electron configuration of atomic (neutral) phosphorous and each of the three ionic states listed above. Clearly label which configuration corresponds to which ion state. **(6 marks)**

Question II: Crystal Structures

1. Show that the atomic packing factor of the hexagonal close-packed structure is 0.74 (assume that c/a = 1.633). **(6 marks)**

2. The density of vanadium (Z=23) is 5.8 g/cm^3. Determine whether vanadium has the face centered cubic or the body centered cubic structure. The unit cell edge length is 0.303 nm and the molar mass is 50.94 g/mol. **(6 marks)**

3. Draw two schematic diagrams of the face centered cubic (FCC) unit cell and indicate the position of the octahedral interstitial positions on one diagram and the tetrahedral interstitial positions on the other. How many interstitial sites of each type are located in the FCC unit cell? **(8 marks)**

Question III: Planes and Directions

1. Draw the following planes in schematic diagrams of the hexagonal close-packed unit cell: (0001), $(10\bar{1}0)$, $(10\bar{1}1)$,and $(11\bar{2}0)$. **(8 marks)**

2. Draw the $[0\bar{1}0]$,$[10\bar{1}]$, and $[1\bar{1}\bar{1}]$ directions for the body centered cubic structure and give the linear densities for each direction. **(6 marks)**

3. Ge has the diamond cubic structure. Calculate the planar densities for the (110) and (111) planes. **(6 marks)**

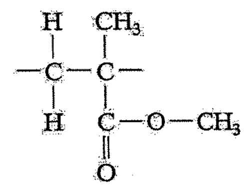
Question IV: Polymer Structures

For a linear polymer molecule, the extended chain length (L_{ext}) depends on the bond length between chain atoms (l), the total number of bonds in the molecule (m), and the angle between adjacent backbone chain atoms (109.5°), as follows:

$$L_{ext} = ml \sin\left(\frac{109.5°}{2}\right)$$

By contrast, the root-mean-square length, $\bar{L}$, is given by: $\bar{L} = l\sqrt{m}$.

1. A linear polymethyl methacrylate (mer unit shown below) polymer has an average molecular weight, $\overline{M}$, of 500,000 g/mole; compute average values of L_{ext} and $\bar{L}$ for this material. The C-C single bond length is 0.154 nm and the C=C double bond length is 0.134 nm. **(10 marks)**

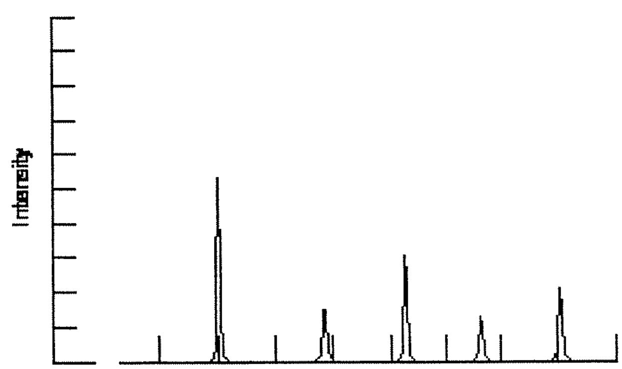


2. Briefly explain the factors which control polymer crystallinity. **(4 marks)**

3. For a linear polypropylene, [-CH_2CHCH_3-]$_n$ determine:
   A) The average molecular weight for L_{ext} = 5000 nm; **(3 marks)**
   B) The average molecular weight for $\bar{L}$ = 30 nm. **(3 marks)**

Question V: X-ray Diffraction

Below is a schematic diagram of the XRD pattern for a BCC material, showing the relative positions of the first five diffraction peaks. Label the diffraction peaks with the (hkl) of the corresponding plane. Note that BCC exhibits diffraction when h+k+l equals an even number. If the atomic radius of this metallic element is 0.125 nm, give the diffraction angle (2θ) of each peak. Assume first order diffraction (n = 1); the wavelength of the X-ray radiation is λ = 0.1542 nm. **(20 marks)**



Question VI: Crystalline Defects -1

1. Briefly explain why the slip direction is $\langle 1\bar{1}0 \rangle$ for dislocations in the FCC crystal structure and $\langle 1\bar{1}1 \rangle$ for dislocations in the BCC crystal structure. **(6 marks)**

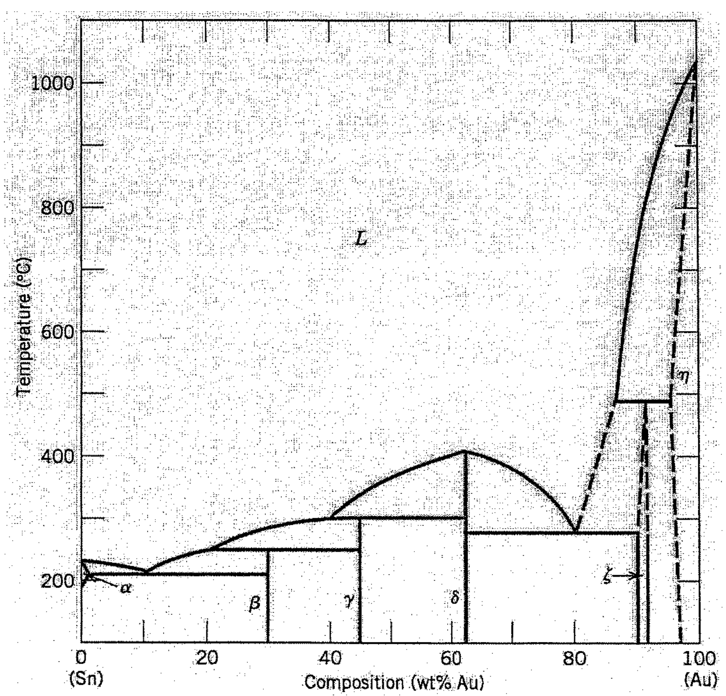
2. What are the two possible slip directions on the BCC (110) slip plane? What is the angle between these directions? **(4 marks)**

3. Briefly explain the differences in the electron band gap structure of intrinsic and extrinsic semiconductors. **(6 marks)**

4. Illustrate a stacking fault in the FCC and HCP crystal structures using the stacking sequence notation, e.g. for a region of perfect FCC crystal: ABCABCABC. **(4 marks)**

Question VII: Phase Diagrams

A region of the Au-Sn equilibrium phase diagram is shown below. For this question assume fully established phase equilibria at any given composition-temperature combination, as established during slow cooling.

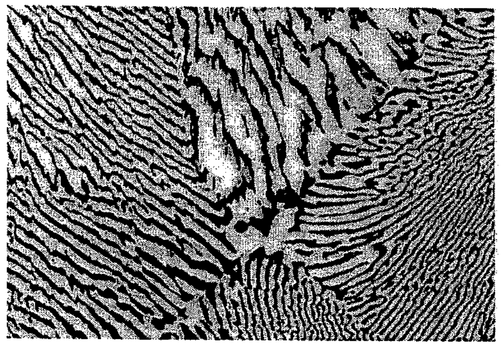


1. Identify all of the invariant reactions shown on this phase diagram, giving their type, the phases involved and the temperature at which they occur. **(10 marks)**

2. Describe the solidification sequence for a Au-5wt.%Sn alloy. **(2 marks)**

3. What is the composition and weight fraction of the phases present for the Sn-70%Au alloy at a temperature of 300°C? **(4 marks)**

4. Shown below is a typical eutectic microstructure. Briefly explain why eutectic microstructures have this characteristic morphology. **(4 marks)**



Question VIII: Crystalline Defects-2

1. Describe three methods in which crystalline defects can be used to increase the strength of a metallic alloy. **(6 marks)**

2. Briefly explain why it is typically more difficult to deform 1) covalently bonded crystals and 2) ionically bonded crystals by dislocation motion than metallic crystals. **(4 marks)**

3. Pb is FCC and has a lattice parameter of a = 0.495 nm. An energy of 0.53 eV/atom is required to produce one vacancy in Pb. Calculate the number of vacancies per m^3 in Pb at 25 °C and at 325 °C. **(10 marks)**

Appendix

Equations and Constants

$$n\lambda = 2d\sin\theta \qquad d = \frac{a}{\sqrt{h^2+k^2+l^2}} \qquad T_K = T_C + 273$$

$$a = 2R \qquad a = 2\sqrt{2}R \qquad a = \frac{4R}{\sqrt{3}} \qquad APF = \frac{V_s}{V_c}$$

$$\rho = \frac{n'\left(\Sigma A_C + \Sigma A_A\right)}{V_C \cdot N_A} \qquad \rho = \frac{n \cdot A}{V_C \cdot N_A} \qquad \frac{n_v}{n_{sites}} = \exp\left(-\frac{E_v}{kT}\right)$$

$$\theta = \cos^{-1}\left[\frac{u_1u_2 + v_1v_2 + w_1w_2}{\sqrt{\left(u_1^2+v_1^2+w_1^2\right)\left(u_2^2+v_2^2+w_2^2\right)}}\right]$$

Atomic Weights:

$A_C = 12.01$ g/mol

$A_H = 1.008$ g/mol

$A_O = 16.00$ g/mol

$A_{Cl} = 35.45$ g/mol

$A_{Fe} = 55.85$ g/mol

Constants:

$k = 1.38 \times 10^{-23}$ J/atom·K

$R = 8.31 J/mol \cdot K$

$e = 1.602 \times 10^{-19} C$

$N_A = 6.023 \times 10^{23} mol^{-1}$